Auxiliary Field Diffusion Monte Carlo calculation of nuclei with $A \leq 40$ with tensor interactions.

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We calculate the ground-state energy of ^{4}He, ^{8}He, ^{16}O, and ^{40}Ca using the auxiliary field diffusion Monte Carlo method in the fixed phase approximation and the Argonne v_6' interaction which includes a tensor force. Comparison of our light nuclei results to those of Green's function Monte Carlo calculations shows the accuracy of our method for both open and closed shell nuclei. We also apply it to ^{16}O and ^{40}Ca to show that quantum Monte Carlo methods are now applicable to larger nuclei.

The nuclear many–body problem has not found a satisfactory solution yet. As opposed to what happens for other systems, one has to face both the absence of a definitive scheme for the description of nucleon–nucleon forces, and with the extreme complexity induced by the fact that forces are state dependent. Recently there have been a few attempts to reduce the problem to a more fundamental level by exploiting in full the scheme of Effective Field Theory (EFT). However, this approach, at present, is applicable only to very small nuclei[1]. Integration of subnuclear degrees of freedom in EFT now provide interactions which are almost as accurate in describing scattering data as the most popular realistic interactions[2]. However, the assessment of the quality of different potentials in many–body sistems remains problematic. Quantum Monte Carlo is the only available tool that provides estimates of physical observables with an accuracy comparable to that obtained by means of few–body techniques [3], but in a wider range of nuclear masses. QMC calculations might therefore help to discuss and gauge the validity of the proposed interactions without the bias implied by the use of approximate methods. However, the operatorial structure of such potentials, both phenomenological and EFT, prevented to push calculations beyond $A = 12$[4]. QMC methods deal with the exponential increase in the computational time with particle number by sampling the degrees of freedom to evaluate sums and integrals. The variational and Green's function Monte Carlo methods[4] are some of the most successful methods for calculating the properties of light nuclei. There the spatial degrees of freedom are sampled, but the spin isospin degrees of freedom of the nucleons are explicitly summed and not sampled. The exponential growth of the spatial degrees of freedom is controlled, but since there are four spin-isospin states per nucleon, the computations grow exponentially – roughly as four raised to the number of nucleons. To make the method computationally efficient, the spin-isospin degrees of freedom must also be sampled. That is what the Auxiliary Field Diffusion Monte Carlo (AFDMC)[5] does in the most efficient way known today.

Here we will demonstrate that AFDMC can be used to solve for the energy of nuclei with nucleons interacting via a somewhat simplified two-body interaction which, however, does contain the tensor interaction that comes from the one-pion exchange potential, and already includes all the terms which make standard approaches unpractical. This interaction term is indeed the most demanding one, together with the short range repulsion, in solving the nuclear many-body Schrödinger equation. Its inclusion in the Hamiltonian provides one of the most severe tests of the efficiency of a quantum Monte Carlo algorithm. Adding the neglected spin-orbit terms and the three-body potential is not expected to change the main conclusion of this paper, namely that AFDMC is applicable with the same accuracy to both nuclei and nuclear matter.

The AFDMC method which includes a path constraint to control the fermion sign problem, has given good results for pure neutron matter[6, 7], for neutron-drops[8] and for the valence neutrons of neutron-rich nuclei[9]. For nuclei, the strong tensor force in the isosinglet channel makes sampling the spin-isospin states more difficult, leading to unsatisfactory results when np and pp interactions are active. In this letter we demonstrate that AFDMC in the fixed phase approximation overcomes this problem, and, as a consequence, can be applied to calculate binding energy of large nuclei and nuclear matter with realistic interactions. Most of our results are with the Argonne v_6' interaction[10], a simplified version of the Argonne v_{18} potential [11] truncated to the first six operators and modified to describe the binding energy of deuteron. We calculate the energy of the alpha particle and the open shell nucleus ^{8}He and test the accuracy of our results by comparing them to those from GFMC[10]. We apply the same algorithm to the study of binding energy of ^{16}O first with the Argonne v_{14} interaction truncated to include only six operators to compare our results

with those of Cluster Variational Monte Carlo[12] and Fermi Hypernetted Chain in the Single Operator Chain approximation (FHNC/SOC). Finally, we calculate, the ground-state energy of the closed-shell nuclei ^{16}O and ^{40}Ca using the Argonne v_6' interaction.

Monte Carlo methods are most efficient when applied to sums and integrals with positive kernels. These can be interpreted as probabilities and probability densities. We have chosen to use the Argonne series of potentials[10] because they are substantially spatially local with only a few derivative terms. The short-time Green's functions that we need are then readily calculated and sampled.

Our Hamiltonian is

$$H = \sum_i \frac{p_i^2}{2m} + \sum_{i<j} \sum_{n=1}^{M} v_n(r_{ij}) O^{(n)}(i,j)$$

where i and j label the two nucleons, r_{ij} is the distance separating the two nucleons, and the $O^{(p)}$ include spin and isospin operators, where M is the number of operators (i.e. 18 in v_{18} models). The mass $m^{-1} = (m_p^{-1} + m_n^{-1})/2$ where m_p and m_n are the proton and neutron masses. We use the Argonne v_6'[10] model where the two-body potential is reprojected from the Argonne v_{18} to the $M = 6$ level. The six $O^{(n)}(i,j)$ terms are the 1, $\vec{\tau}_i \cdot \vec{\tau}_j$, $\vec{\sigma}_i \cdot \vec{\sigma}_j$, $(\vec{\sigma}_i \cdot \vec{\sigma}_j)(\vec{\tau}_i \cdot \vec{\tau}_j)$, S_{ij}, and $S_{ij} \vec{\tau} \cdot \vec{\tau}_j$, where S_{ij} is the tensor operator $3\vec{\sigma}_i \cdot \hat{r}_{ij} \vec{\sigma}_j \cdot \hat{r}_{ij} - \vec{\sigma}_i \cdot \vec{\sigma}_j$. The $\vec{\tau}_i$ and $\vec{\sigma}_i$ are the Pauli matrices for the isospin and spin of particle i. The inclusion of neutron-proton mass difference, electromagnetic interactions, spin-orbit interactions, and three-body potentials can be done with an increase in complexity. However the bulk of the binding energy comes from the v_6 terms which include the one-pion exchange parts of the potential.

Traditionally, ground-state quantum Monte Carlo calculations begin by using a variational calculation to optimize a trial wave function. This trial wave function is then used to guide the sampling of the random walk in diffusion or Green's function Monte Carlo. A typical form for a good trial function has a model function $|\Phi\rangle$ given by a small linear combination of antisymmetric products of orbitals multiplied by a symmetrized product of two-body operator correlations. Evaluating this symmetrized product trial function at the spatial positions R and spin-isospin values S gives the expression

$$\langle R,S|\Psi_{SP}\rangle = \langle R,S|\mathcal{S}\prod_{i<j}\left[\sum_{p=1}^{M} f^{(p)}(r_{ij})O^{(p)}(i,j)\right]|\Phi\rangle\,. \tag{1}$$

Unfortunately, the evaluation of this wave function requires exponentially increasing computational time with the number of particles. Since the evaluation for all spin-isospin values has the same computational complexity, light nuclei variational and Green's function Monte Carlo calculations sum the spin-isospin degrees of freedom.

Since for large numbers of particles we cannot evaluate these trial functions, we use much simpler wave functions which contain only the central Jastrow correlation. The evaluation of our simpler wave function require order A^3 operations to evaluate the Slater determinants and A^2 operations for the central Jastrow. Since many important correlations are neglected in these simplified functions, we use the Hamiltonian itself to define the spin sampling.

Specifically our trial function is

$$\langle RS|\Psi_T\rangle = \left[\prod_{i<j} f_{ij}^c\right] \mathcal{A}\left[\prod_i \phi_i(\vec{r}_i - R_{\rm cm}, s_i)\right]\,. \tag{2}$$

where $\mathcal{A}$ is an antisymmetrization operator, ϕ are single particle space and spin-isospin orbitals, built from combinations of radial functions, spherical harmonics and spinors. $R_{\rm cm} = A^{-1}\sum_{i=1}^{A}\vec{r}_i$ is the center of mass of the nucleus. The Jastrow function is the central part of the FHNC/SOC[13] correlation operator $\hat{F}_{ij}$ which minimized the energy of nuclear matter at ρ_0=0.16 fm^{-3}.

Radial orbitals are calculated in the self-consistent potential generated by the Hartree-Fock algorithm with Skyrme's effective interactions of Ref. [14] that has been used to study light nuclei. Given a set of positions and spinors, the antisymmetrization produces a determinant of single particle orbitals. For open-shell nuclei, a sum of several determinants is used to build a trial wavefunction of a total angular momentum J that describes the nucleus. The determinants are multiplied by the central Jastrow factor to give the value of our trial function.

The AFDMC method works much like diffusion Monte Carlo[5, 6, 8, 9]. The wave function is defined by a set of what we call walkers. Each walker is a set of the $3A$ coordinates of the particles plus A normalized four component spinors representing the spin-isospin state. The imaginary time propagator for the kinetic energy and the spin-independent part of the potential is identical to that used in standard diffusion Monte Carlo. The new positions are sampled from a drifted Gaussian with a weight factor for branching given by the local energy of these components. Since these parts do not change the spin state, the spinors will be unchanged by these parts of propagator.

To sample the spinors we first use a Hubbard Stratonovich transformation to write the propagator as an integral over auxiliary fields of a separated product of single particle spin-isospin operators. We then sample the auxiliary field value, and the resulting sample independently changes each spinor for each particle in the sample, giving a new sampled walker.

Specifically we write the v_6 interaction as

$$\begin{aligned} V &= \sum_{i<j} v_1(r_{ij}) + V_{sd} \\ V_{sd} &= \frac{1}{2}\sum_{i\alpha,j\beta}\sigma_{i\alpha}A^{(\sigma)}_{i\alpha,j\beta}\sigma_{j\beta} + \frac{1}{2}\sum_{i\alpha,j\beta}\sigma_{i\alpha}A^{(\sigma\tau)}_{i\alpha,j\beta}\sigma_{j\beta}\vec{\tau}_i\cdot\vec{\tau}_j \end{aligned}$$

$$+ \ \frac{1}{2}\sum_{i,j} A^{(\tau)}_{i,j}\vec{\tau}_i\cdot\vec{\tau}_j. \qquad (3)$$

Where $v_1(r)$ is the central interaction, and V_{sd} is the spin-isospin dependent part. The A matrices depend only on the positions of the particles. They are zero when $i=j$ and they are real and symmetric so that they have real eigenvalues $\lambda^{(\sigma)}_n$, $\lambda^{(\sigma\tau)}_n$, $\lambda^{(\tau)}_n$ and corresponding real normalized eigenvectors $\psi^{(\sigma)}_n(i,\alpha)$, $\psi^{(\sigma\tau)}_n(i,\alpha)$,$\psi^{(\tau)}_n(i)$. The spin-dependent potential can be written as a sum of squares of single-particle operators as

$$V_{sd} \ = \ \frac{1}{2}\sum_{m=1}^{15A}\lambda_m O_m^2 \qquad (4)$$

where the $15A$ operators

$$\begin{aligned} O^{(\sigma)}_n &= \sum_{i\alpha}\sigma_{i\alpha}\psi^{(\sigma)}_n(i,\alpha) \\ O^{(\sigma\tau)}_{n\alpha} &= \sum_{i\beta}\tau_{i\alpha}\sigma_{i\beta}\psi^{(\sigma\tau)}_n(i,\beta) \\ O^{(\tau)}_{n\alpha} &= \sum_{i}\tau_{i\alpha}\psi^{(\tau)}_n(i) \end{aligned} \qquad (5)$$

are labeled in a convenient order of the eigenvectors and the corresponding eigenvalues.

We apply the Hubbard-Stratonovich transformation to write

$$e^{-\frac{1}{2}\Delta t\lambda O^2} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx e^{-\frac{x^2}{2}+\sqrt{-\lambda\Delta t}xO}, \qquad (6)$$

where x is an auxiliary field. Each of the 15A terms in Eq. 4 requires an auxiliary field. We write the short time approximation of the spin-dependent propagator as

$$e^{-V_{sd}\Delta t} = \int dX \exp\left[-\sum_{n=1}^{15A}\left(\frac{x_n^2}{2} - x_n\sqrt{-\lambda_n\Delta t}O_n\right)\right] \qquad (7)$$

where $dX \equiv \prod_{n=1}^{15A}\frac{dx_n}{\sqrt{2\pi}}$ and we drop commutator terms which are higher order than Δt on the right hand side.

Once the Hubbard-Stratonovich variables have been sampled, the resulting propagator acting on a walker (i.e. positions and spinors) gives a single new walker.

Since the trial function evaluated at the walker spin-isospin and position can be complex, we use a fixed-phase approximation[15]. We importance sample the auxiliary field variables x_m by writing

$$\begin{aligned} &\frac{x_n^2}{2} + x_n\sqrt{-\lambda_n\Delta t}O_n \\ &= \frac{x_n^2}{2} + x_n\sqrt{-\lambda_n\Delta t}\langle O_n\rangle + x_n\sqrt{-\lambda_n\Delta t}(O_n - \langle O_n\rangle) \end{aligned} \qquad (8)$$

where $\langle O_n\rangle = \langle\Psi_T|O_n|R,S\rangle/\langle\Psi_T|R,S\rangle$ is the mixed expectation value. The first two terms are then combined to form a shifted contour Gaussian as in Ref. [16]. Applying the fixed phase approximation, instead of the previously used constrained path, the walker weight can be reexpressed in terms of the local energy

$$E_L(R,S) = \mathrm{Re}\frac{\langle\Psi_T|H|RS\rangle}{\langle\Psi_T|RS\rangle}. \qquad (9)$$

This change to the original algorithm was necessary to overcome the unphysical discrepancies observed in earlier AFDMC work on nuclei with tensor forces [17].

Our algorithm becomes: i) sample $|R,S\rangle$ initial walkers from $|\langle\Psi_T|R,S\rangle|^2$ using Metropolis Monte Carlo; ii) propagate in the usual DMC way with a drifted Gaussian for a time step; iii) diagonalize, for each walker, the potential matrices $A^{(\sigma)}$, $A^{(\tau)}$ and $A^{(\sigma\tau)}$; iv) sample the corresponding shifted contour auxiliary field variables and update the spinors. The new walker has a weight given by $\exp(-E_L(R',S')\Delta t)$.

Our trial function contains no tensor correlations and the variational estimate is not even bound. The diffusion process enforced by the AFDMC method is capable of crossing the transition from an unbound to a bound system, leading to energy estimates which compare very well with the available GFMC results. Table I reports results for the alpha particle and the open shell nucleus ^{8}He. For the alpha particle AFDMC estimates are compared with GFMC and the Effective Interaction Hyperspherical Harmonic (EIHH) methods[20]. The AFDMC agreement with GFMC and EIHH for ^{4}He is within about 1% of the total energy. The agreement between AFDMC and GFMC for ^{8}He is even better.

TABLE I: The Ground-State energies of the alpha particle and of ^8He calculated with different methods using the Argonne v_6' interaction. The GFMC results are taken from Ref. [10] after the subtraction of the Coulomb term of 0.7MeV[18]. The EIHH result[19] doesn't contain the Coulomb interaction. All the value are expressed in MeV.

method	$E(^4\mathrm{He})$	$E(^8\mathrm{He})$
AFDMC	-27.13(10)	-23.6(5)
GFMC	-26.93(1)	-23.6(1)
EIHH	-26.85(2)	

We have compared our results for ^{16}O with other methods. The variational FHNC/SOC[21], and Cluster variational calculations[12] used the Argonne v_{14} interaction. Our result for the energy, keeping just the first six operators, is -90.8(1) MeV. The variational results keeping just those same six operators are -83.2 MeV from Variational Monte Carlo and -84.0 MeV from FHNC/SOC. The AFDMC method seems to lower the energy by about 10% with respect to the two different variational results; however, the variational wavefunctions were optimized with the full v_{14} interaction instead of our truncated interaction.

TABLE II: Computed Ground-State Energy in MeV of ^{4}He, ^{8}He, ^{16}O and ^{40}Ca for the Argonne v_6' interaction. Experimental energies are also reported[22]. We also calculated the energy of 28 nucleons in a periodic box to extrapolated the nuclear matter energy at equilibrium density as described in Ref. [23] All the value are expressed in MeV.

nucleus	E	E/A	E_{exp}	E_{exp}/A
^{4}He	-27.20(5)	-6.8	-28.296	-7.074
^{8}He	-23.6(5)	-2.95	-31.408	-3.926
^{16}O	-100.7(4)	-6.29	-127.619	-7.98
^{40}Ca	-272(2)	-6.8	-342.051	-8.55
nuclear matter		-12.8(1)		

We then performed calculations for the ^{16}O and for ^{40}Ca with the Argonne v_6' NN interaction. We chose this potential because it is a reprojected version of the more sophisticated Argonne v_{18}. Its main deficiency is the lack of a spin-orbit interaction and the three-body potential.

Results are reported in table II, where it is reported also the energy of nuclear matter at the equilibrium density ρ_0=0.16fm^{-3} calculated with AFDMC[23].

As expected the v_6' interactions is not sufficient to build the total binding energy of ^{16}O and of ^{40}Ca. This NN interaction gives about 96% of total binding energy for alpha particle, 75% for ^{8}He, 79% for ^{16}O and 79% for ^{40}Ca. Our ^{16}O is unstable to break up into 4 alpha particles, and our ^{40}Ca has the same energy of 10 alpha particles. This is behavior is consistent with the simple pair counting argument of Ref. [24]. The surface energy coefficient in the Weizsacker formula, resulting from the comparison of the binding energies per nucleon of symmetrical nuclear matter and ^{40}Ca is 20.5 MeV, not too far from the experimental value of 18.6 MeV.

We have extended the AFDMC method, used to perform calculations for neutron systems, to study finite nucleonic systems and have obtained agreement with results from other methods for light nuclei. The method easily accommodates open-shell nuclei. We have calculated systems with up to A=40 nucleons here. The computational time per imaginary time step scales as A^3. The total computational time depends on the desired quantity, the distribution of excited states, and the quality and complexity of the trial function just as in all other quantum Monte Carlo methods. We believe that the results we have presented show that AFDMC in the fixed phase approximation has become a very powerful tool to solve large nuclear systems with realistic interactions. This opens up the possibility of calculating at an enriched accuracy heavy nuclei and asymmetric nuclear matter.

To be able to predict accurately the structure of nuclei, we must use a more realistic Hamiltonian. The main two features missing from this work are the three-body potential and spin orbit terms.

The Urbana-IX potential has been used by us in previous neutron studies. This potential contains a spin-independent short range repulsion, and operator terms based on the Fujita-Miyazawa model. The spin-independent part and the so-called anticommutator terms lead to terms with two- or fewer spin-isospin operators and can be included immediately in AFDMC calculations. The commutator terms have as well as the isospin exchange spin-orbit require additional auxiliary fields to rewrite them in terms of single-particle spin-isospin operators. The other terms in a more realistic interaction are included perturbatively in GFMC calculations. Initially, we will also try to include them perturbatively. This will likely be more difficult in AFDMC than in GFMC since our trial wave functions are much simpler and much less accurate so that the perturbative estimates will likely also be less accurate. The inclusion of these terms is in progress and will be the subject of future works.

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